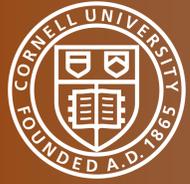


HIGH-FIDELITY NUMERICAL MODELING OF SPRAY DROPLET FORMATION

2023 IFPRI ANNUAL GENERAL MEETING



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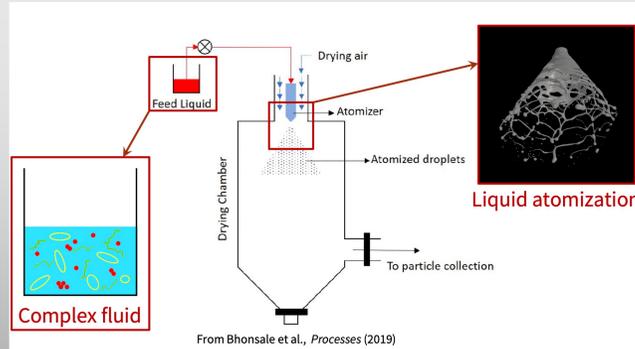
Motivation

- Many industrial processes such as spray drying for powder production rely on **atomizing complex fluids** into a spray
- Complex liquid rheology adds significant challenges** to a phenomenon that is already challenging to model and predict
- Assess and enhance ability of our novel high-fidelity multiscale spray atomization model for complex fluids

Objective

- Assess influence of high viscosity fluid in pressure swirl configuration
- Identify experimental datasets for complex fluid atomization
- Implemented non-Newtonian model in flow solver

Accomplishments



Complex fluid phenomena

- High effective viscosity, shear-rate-dependent viscosity, viscoelasticity, viscoplasticity, etc...

Polymeric fluids

Resulting non-Newtonian behavior in the fluid

- Shear generates pseudo elastic polymeric stresses \Rightarrow **Viscoelastic**
- Shear lowers effective fluid viscosity \Rightarrow **Shear-thinning**

Deborah number $De = \frac{\text{Polymer relaxation time}}{\text{Flow characteristic time}} = \frac{\lambda}{t_f}$

Deborah number $\gg 1$: solid-like behavior
Deborah number $\ll 1$: fluid-like behavior

Pressure-swirl atomization

Newtonian: $Re_l = 100, We_l = 1000$

laminar inlet

numerical tearing due to insufficient resolution

Newtonian: $Re_l = 5000, We_l = 1000$

interface disrupted by inlet turbulence

hole formation

hole growth via rim retraction

ligament formation

ligament break-up via Rayleigh-Plateau

Mathematical model

Continuity: $\nabla \cdot \mathbf{u} = 0$

Liquid volume conservation: $\frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \nabla \alpha = 0$

Momentum conservation: $\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \nabla \cdot \boldsymbol{\tau}_p + \nabla \cdot \boldsymbol{\tau}_{sgs} + \mathbf{F}_{ST}$

Viscous stresses – Carreau model

$\boldsymbol{\tau} = 2\mu \mathbf{S}$

$\rho = \alpha \rho_l + (1 - \alpha) \rho_g$

$\mu = \alpha \mu_l + (1 - \alpha) \mu_g$

$\mu_l = \mu_s + \mu_p$ with $\mu_p = \mu_{p,0} (1 + (\lambda S)^2)^{\frac{n-1}{2}}$

Elastic stresses – FENE-CR model

- Elastic dumbbells model of polymers
- Represents a Boger fluid
- \mathbf{C} = conformation tensor and \mathbf{I} = identity tensor
- \mathbf{C} and \mathbf{C} is solution of

$\frac{\partial \mathbf{C}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{C} = \nabla \mathbf{u} \cdot \mathbf{C} + \mathbf{C} \cdot (\nabla \mathbf{u})^T - f \frac{\mathbf{C} - \mathbf{I}}{\lambda}$

No atomization in domain

Atomization partially captured in domain

Experimental results from Ashgriz IFPRI Final Report FRR-96-05 (2022):

60% Glycerin, $Re_l \sim 4500$

@ nozzle exit

@ 5 mm downstream

Bag break-up of ligament

$We_l^{exp} \approx 10 We_l^{sim}$

Shear-thinning: $Re_l = 1000, We_l = 500, n = 1/2, \lambda D/U = 10$

Annular pipe is fully turbulent

Low viscosity due to high shear in nozzle \Rightarrow Turbulent inlet \Rightarrow Hole formation

Low viscosity around retracting rims

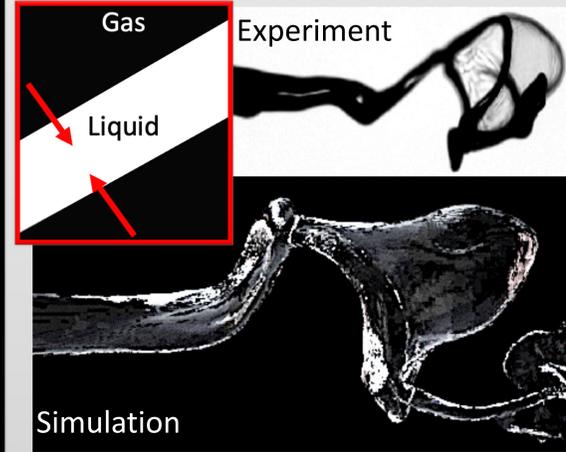
λS

$\mu_l(S)/\mu_g$

Ongoing model development

Sub-grid tracking of interfacial structures

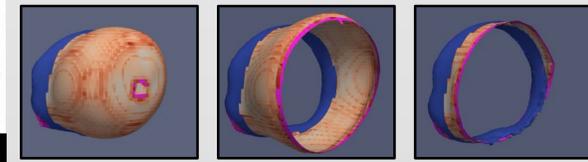
- Interface reconstruction with two planes in each cell maintains sub-grid-thickness films



Sub-grid scale breakup modeling

- Films are detected and are treated with two possible models

1. Undergo Taylor-Culick retraction

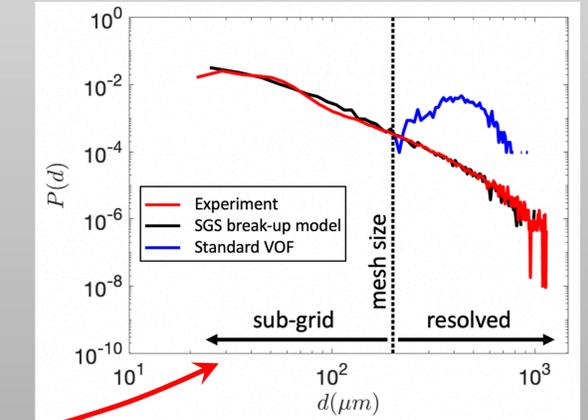
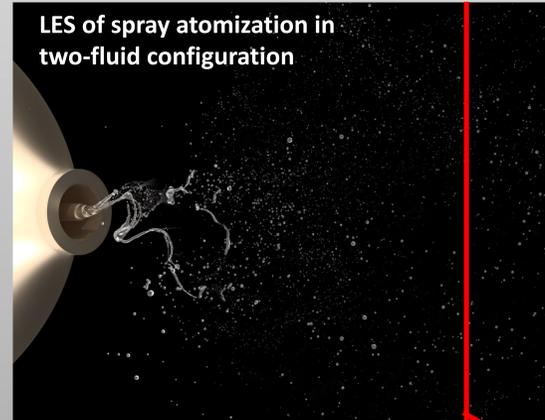


2. Undergo instantaneous bursting



High-fidelity multiscale modeling of atomization

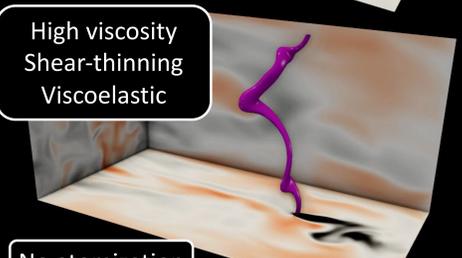
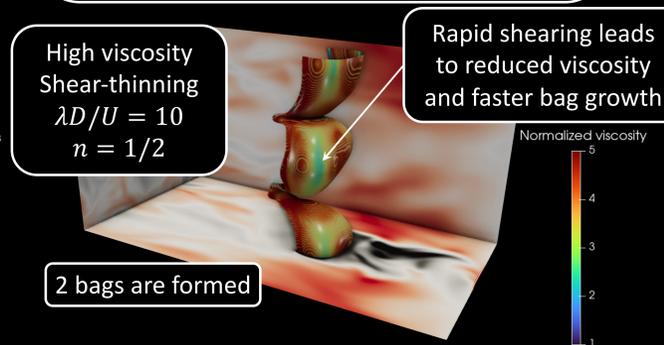
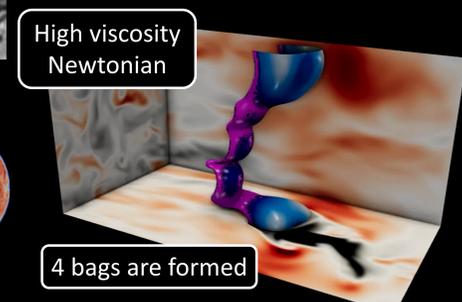
- Recently developed multiscale modeling framework for spray atomization shows promise for mesh-independent drop size predictions



Isolated ligament break-up in a cross-flow

Model	μ_l/μ_g	ρ_l/ρ_g
Newtonian	50	1000
Newtonian	500	1000
Shear-thinning	500	1000
Shear-thinning and viscoelastic	500	1000

- Liquid ligament is accelerated by gas \Rightarrow Susceptible to **Rayleigh-Taylor instability**
- Most unstable wavelength given by $\frac{\lambda_{RT}}{D} = \sqrt{\frac{6\pi^3 \rho_l}{C_D (\rho_l - \rho_g)}} We_g^{-1/2}$
- Inviscid theory predicts **6 bags in simulation**



Future steps

- Further validation of complex, viscoelastic fluid models
- Quantitative comparison examining the impact of high viscosity and complex rheology:
 - Pressure swirl atomization
 - Isolated ligament in turbulent cross flow